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Evaluation of Reflection Boundary Conditions for Langevin Equation Modeling of Convective Boundary Layer Dispersion

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ABSTRACT

Reflection boundary conditions for a Lagrangian stochastic particle model of vertical dispersion in the convective boundary layer, CBL, are evaluated using simulations of well-mixed position and velocity distributions, and simulations of the cross-wind-integrated air concentration from Willis and Deardorff's (1976, 1978, 1981) water tank experiments. The model is based on a Langevin equation with the assumption that the turbulent properties of the CBL (skewness, variance, and Lagrangian correlation time scale of the vertical velocity) are vertically homogeneous and representative of the bulk of the CBL, the mixed layer. In this model, the surface and free convection layers near the bottom boundary and the entrainment layer at the top of the CBL are not resolved. The advantage of these assumptions is that considerably longer time steps may be used in numerical simulations, while still retaining the essential statistical properties of the vertical velocity that affect CBL dispersion: the skewness of the vertical velocity distribution and the long velocity correlation time scale. Hurley and Physick (1993) used similar assumptions about homogeneous turbulent properties in Langevin equation model simulations of water tank dispersion experiments and obtained reasonable results. The choice of reflection boundary condition (i.e., the method used to determine a new velocity for a particle that encounters a boundary) is more important in this type of model, compared to models assuming inhomogenous turbulence (with velocity variance and/or time scale becoming small near boundaries), because there are more "collisions" with the boundary, and they occur with higher magnitude velocities.

Hurley and Physick's simulations and all other previous Langevin equation simulations of CBL dispersion have made use of reflection methods in which the magnitudes of the incident and reflected velocities were positively correlated. In addition, a limitation of previous Langevin equation simulations of CBL dispersion is that the reflection methods used were unable to maintain a well-mixed position and velocity distribution in skewed, homogenous turbulence, as discussed by several previous investigators (e.g., Wilson and Flesch, 1993; Hurley and Physik, 1993; Thomson and Montgomery, 1994). Thomson and Montgomery (1994) presented a sound basis for deriving reflection methods, and tested one successful method (with positively correlated speeds) versus a vertically-well-mixed steady-state particle position distribution. We evaluate and compare three methods based on the Thomson and Montgomery approach using simulations of well-mixed position and

velocity distributions, and of CBL water tank experiments. In addition to a method using the standard assumption that incident and reflected speed are positively correlated, we evaluate and compare two other methods which may be more realistic, and in which (1) the incident and reflected speed are negatively correlated, and (2) the reflected velocity is chosen randomly from the proper distribution. We discuss the results from these three methods in light of the observed structure of CBL circulations.

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